wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 05:31 PM EDT

PDB ID	:	6UC1
Title	:	Crystal structure of D678A GoxA soaked in glycine at pH 7.5
Authors	:	Yukl, E.T.
Deposited on	:	2019-09-13
Resolution	:	2.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

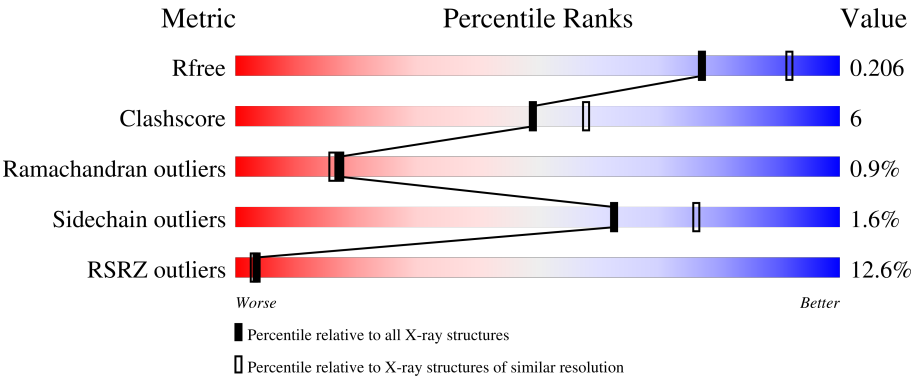
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	816	14% 82% 11% • 5%
1	B	816	10% 85% 9% • 5%
1	D	816	13% 82% 12% • 5%
2	C	816	11% 82% 12% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GLY	D	905	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 49336 atoms, of which 23369 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Uncharacterized protein GoxA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	776	Total	C	H	N	O	S	0	0	0
			11936	3880	5803	1044	1189	20			
1	A	776	Total	C	H	N	O	S	0	1	0
			12010	3889	5866	1044	1191	20			
1	D	776	Total	C	H	N	O	S	0	2	0
			11992	3890	5844	1047	1191	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ALA	ASP	engineered mutation	UNP A0A161XU12
A	678	ALA	ASP	engineered mutation	UNP A0A161XU12
D	678	ALA	ASP	engineered mutation	UNP A0A161XU12

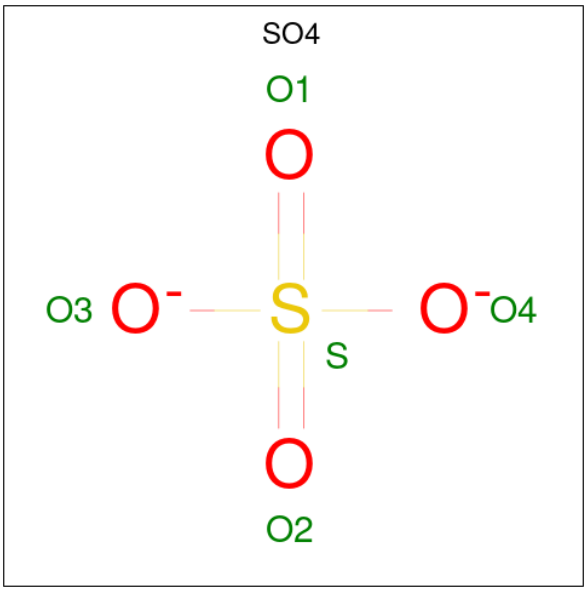
- Molecule 2 is a protein called Uncharacterized protein GoxA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	777	Total	C	H	N	O	S	0	0	0
			11971	3892	5822	1046	1192	19			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	678	ALA	ASP	engineered mutation	UNP A0A161XU12

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

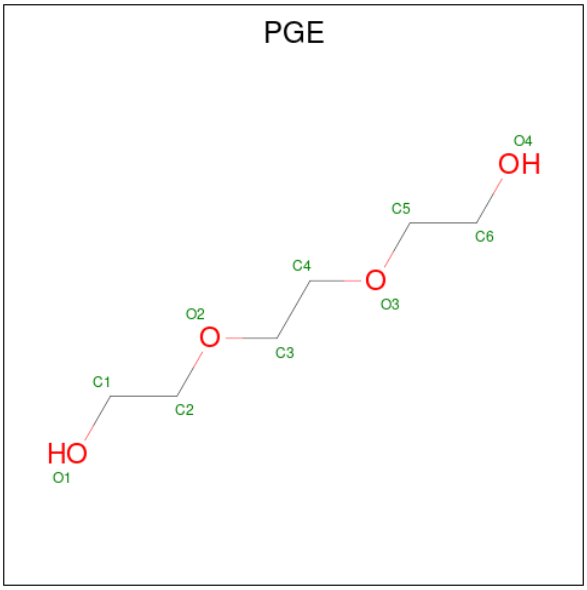


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

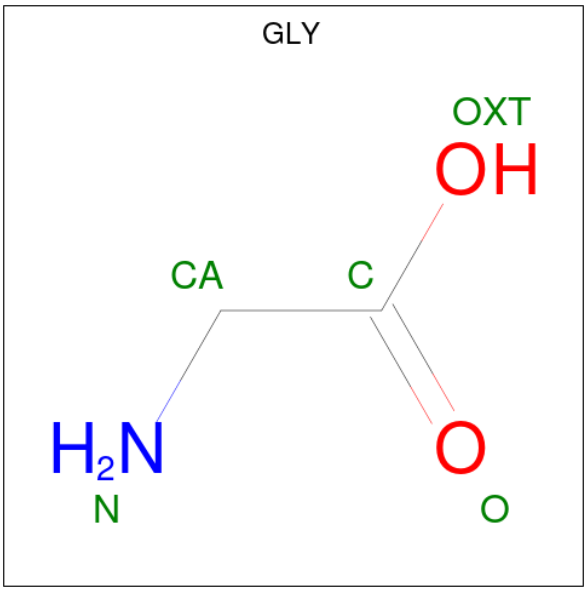
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 24 6 14 4	0	0

- Molecule 6 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O 10 2 5 1 2	0	0
6	A	1	Total C H N O 10 2 5 1 2	0	0
6	D	1	Total C H N O 10 2 5 1 2	0	0
6	D	1	Total C H N O 10 2 5 1 2	0	0

- Molecule 7 is water.

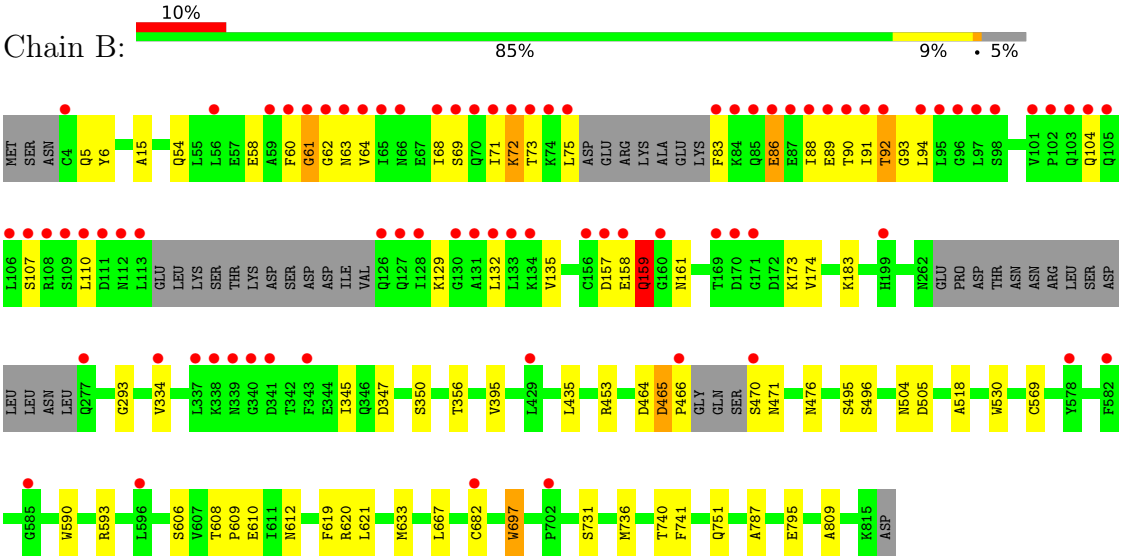
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	365	Total O 366 366	0	1
7	A	288	Total O 288 288	0	0
7	D	269	Total O 269 269	0	0
7	C	376	Total O 376 376	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

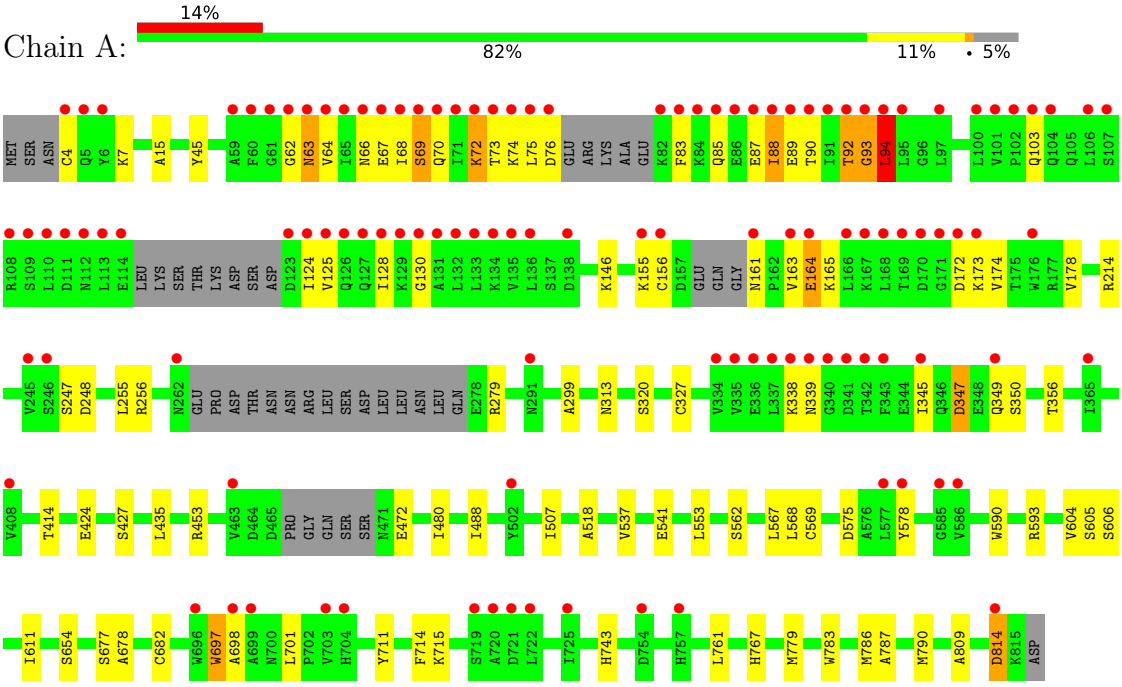
• Molecule 1: Uncharacterized protein GoxA

Chain B:



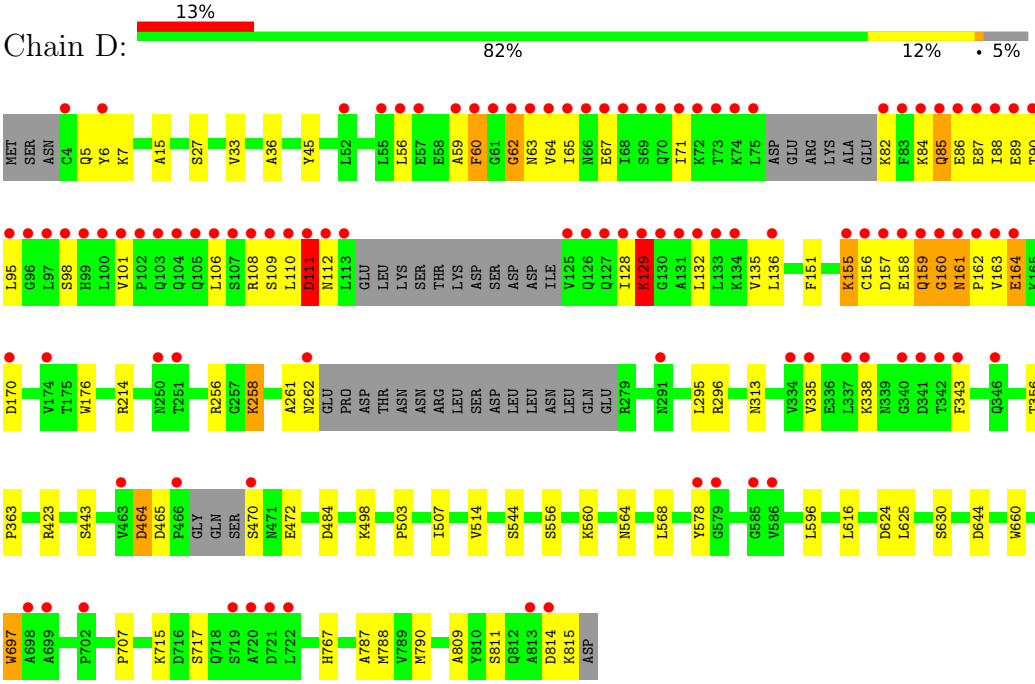
• Molecule 1: Uncharacterized protein GoxA

Chain A:



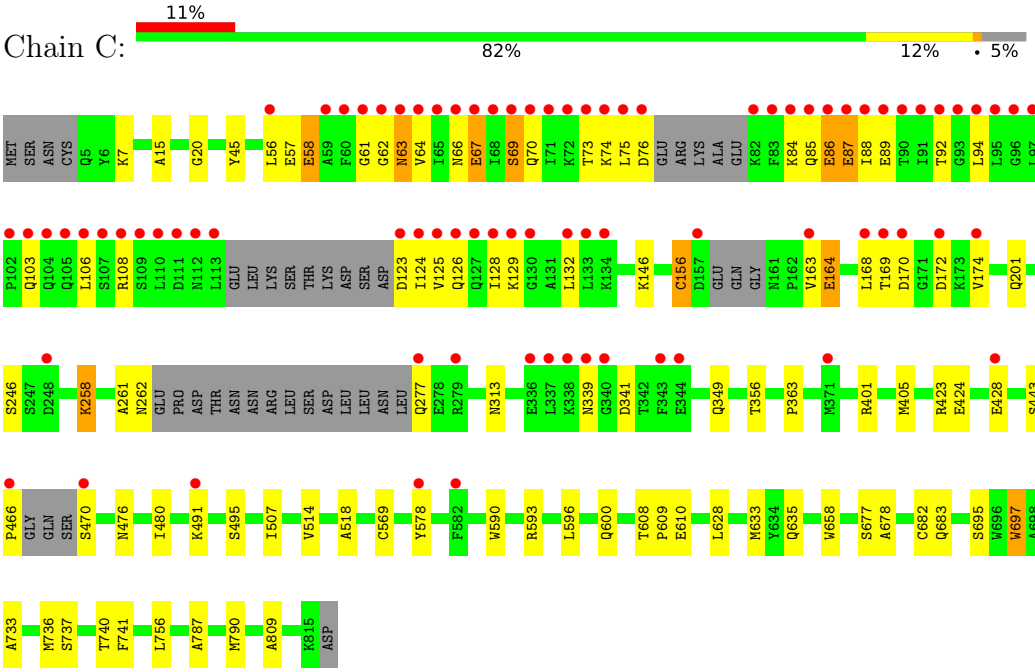
• Molecule 1: Uncharacterized protein GoxA

Chain D:



• Molecule 2: Uncharacterized protein GoxA

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.21Å 93.53Å 188.33Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	48.38 – 2.19 48.38 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-2.19) 99.4 (48.38-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.169 , 0.206 0.170 , 0.206	Depositor DCC
R_{free} test set	9756 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	49336	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, PGE, TRQ, Q3P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.53	1/6273 (0.0%)	0.59	2/8536 (0.0%)
1	B	0.56	1/6264 (0.0%)	0.62	1/8526 (0.0%)
1	D	0.46	0/6279	0.57	0/8546
2	C	0.53	2/6265 (0.0%)	0.62	2/8526 (0.0%)
All	All	0.52	4/25081 (0.0%)	0.60	5/34134 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	CYS	CB-SG	-18.59	1.50	1.82
1	B	173	LYS	CE-NZ	-14.19	1.13	1.49
2	C	69	SER	CB-OG	-6.21	1.34	1.42
2	C	156	CYS	CB-SG	-5.38	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	173	LYS	CD-CE-NZ	-11.47	85.33	111.70
2	C	69	SER	CB-CA-C	-6.40	97.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	814	ASP	CB-CG-OD2	6.35	124.02	118.30
2	C	790	MET	CG-SD-CE	6.35	110.36	100.20
1	A	347	ASP	CB-CG-OD1	-5.48	113.37	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	LEU	Peptide
1	B	86	GLU	Peptide
1	D	111	ASP	Peptide
1	D	159	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6144	5866	5917	73	1
1	B	6133	5803	5905	65	1
1	D	6148	5844	5923	80	0
2	C	6149	5822	5910	69	0
3	A	10	0	0	1	0
3	B	25	0	0	2	0
3	C	15	0	0	1	0
3	D	10	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	10	14	14	0	0
6	A	10	10	4	3	0
6	D	10	10	4	3	0
7	A	288	0	0	8	0
7	B	366	0	0	1	0
7	C	376	0	0	4	0
7	D	269	0	0	5	0
All	All	25967	23369	23677	287	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 287 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLN:NE2	1:B:58:GLU:OE1	1.84	1.09
1:D:644:ASP:OD2	7:D:1001:HOH:O	1.79	0.98
2:C:86:GLU:HB3	2:C:89:GLU:HB2	1.48	0.94
1:B:334:VAL:O	7:B:1001:HOH:O	1.86	0.91
2:C:75:LEU:HD21	2:C:87:GLU:OE1	1.71	0.90

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLY:N	1:A:67:GLU:OE2[1_455]	1.96	0.24

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	764/816 (94%)	719 (94%)	35 (5%)	10 (1%)	12 9
1	B	765/816 (94%)	735 (96%)	25 (3%)	5 (1%)	22 22
1	D	767/816 (94%)	726 (95%)	33 (4%)	8 (1%)	15 14
2	C	763/816 (94%)	728 (95%)	31 (4%)	4 (0%)	29 31
All	All	3059/3264 (94%)	2908 (95%)	124 (4%)	27 (1%)	17 16

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	GLY

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Mol	Chain	Res	Type
1	B	159	GLN
1	A	94	LEU
1	D	60	PHE
1	D	111	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	673/710 (95%)	664 (99%)	9 (1%)	69 81
1	B	672/710 (95%)	666 (99%)	6 (1%)	78 88
1	D	674/710 (95%)	659 (98%)	15 (2%)	52 65
2	C	673/709 (95%)	660 (98%)	13 (2%)	57 71
All	All	2692/2839 (95%)	2649 (98%)	43 (2%)	62 76

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	715	LYS
2	C	246	SER
1	D	717	SER
2	C	86	GLU
2	C	423	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	103	GLN
2	C	718	GLN
2	C	112	ASN
2	C	600	GLN
1	A	127	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TRQ	C	697	2	13,17,18	1.84	4 (30%)	14,24,26	2.18	5 (35%)
1	TRQ	A	697	1	13,17,18	1.81	4 (30%)	14,24,26	1.97	4 (28%)
1	TRQ	D	697	1	13,17,18	1.75	4 (30%)	14,24,26	1.70	3 (21%)
2	Q3P	C	222	2	10,12,13	0.93	0	5,13,15	0.79	0
1	TRQ	B	697	1	13,17,18	1.78	3 (23%)	14,24,26	1.94	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	C	697	2	-	0/4/19/21	0/2/2/2
1	TRQ	A	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	D	697	1	-	0/4/19/21	0/2/2/2
2	Q3P	C	222	2	-	2/11/12/14	-
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	697	TRQ	CB-CG	-4.27	1.45	1.51
2	C	697	TRQ	CE2-CZ2	-4.27	1.44	1.50
1	B	697	TRQ	CE2-CZ2	-2.98	1.46	1.50
1	A	697	TRQ	CE2-CZ2	-2.97	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CB-CG	-2.86	1.47	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	697	TRQ	CZ2-CE2-NE1	4.77	127.55	119.94
1	B	697	TRQ	CZ2-CE2-NE1	4.46	127.06	119.94
1	A	697	TRQ	CZ2-CE2-NE1	4.30	126.80	119.94
2	C	697	TRQ	O6-CH2-CZ2	-3.75	115.96	118.51
2	C	697	TRQ	CZ2-CE2-NE1	3.72	125.87	119.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	222	Q3P	O2-C1-C4-N5
2	C	222	Q3P	NZ-C1-C4-N5

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	697	TRQ	3	0
1	A	697	TRQ	2	0
1	D	697	TRQ	1	0
1	B	697	TRQ	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PGE	B	907	-	9,9,9	0.39	0	8,8,8	0.25	0
3	SO4	B	905	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	B	903	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	B	902	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	B	904	-	4,4,4	0.12	0	6,6,6	0.15	0
3	SO4	A	901	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	C	903	-	4,4,4	0.19	0	6,6,6	0.19	0
6	GLY	D	905	-	4,4,4	1.26	1 (25%)	3,4,4	1.88	1 (33%)
3	SO4	A	902	-	4,4,4	0.13	0	6,6,6	0.08	0
3	SO4	D	902	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	C	902	-	4,4,4	0.19	0	6,6,6	0.08	0
3	SO4	B	901	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	C	901	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	D	901	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GLY	A	905	-	4,4,4	1.04	0	3,4,4	1.41	0
6	GLY	A	904	-	4,4,4	1.11	1 (25%)	3,4,4	1.69	1 (33%)
6	GLY	D	904	-	4,4,4	1.13	1 (25%)	3,4,4	1.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	B	907	-	-	2/7/7/7	-
6	GLY	D	904	-	-	0/2/2/2	-
6	GLY	D	905	-	-	2/2/2/2	-
6	GLY	A	905	-	-	2/2/2/2	-
6	GLY	A	904	-	-	0/2/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	905	GLY	OXT-C	-2.41	1.22	1.30
6	D	904	GLY	OXT-C	-2.14	1.23	1.30
6	A	904	GLY	OXT-C	-2.13	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	905	GLY	OXT-C-O	-2.61	116.80	123.30
6	A	904	GLY	OXT-C-CA	2.08	121.74	113.45

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	905	GLY	O-C-CA-N
6	A	905	GLY	OXT-C-CA-N
6	D	905	GLY	O-C-CA-N
6	D	905	GLY	OXT-C-CA-N
5	B	907	PGE	O2-C3-C4-O3

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	904	SO4	1	0
3	A	901	SO4	1	0
6	D	905	GLY	1	0
3	D	902	SO4	1	0
3	B	901	SO4	1	0
3	C	901	SO4	1	0
6	A	905	GLY	1	0
6	A	904	GLY	2	0
6	D	904	GLY	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	775/816 (94%)	0.84	116 (14%) 2 2	26, 48, 114, 150	0
1	B	775/816 (94%)	0.63	79 (10%) 6 6	22, 38, 102, 162	0
1	D	775/816 (94%)	0.83	110 (14%) 2 2	25, 49, 121, 156	0
2	C	775/816 (94%)	0.68	87 (11%) 5 4	21, 39, 105, 142	0
All	All	3100/3264 (94%)	0.75	392 (12%) 3 3	21, 44, 111, 162	0

The worst 5 of 392 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	12.7
2	C	65	ILE	12.5
1	D	113	LEU	11.1
1	A	83	PHE	10.6
2	C	88	ILE	10.1

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	Q3P	C	222	13/14	0.93	0.14	24,34,79,94	0
1	TRQ	A	697	16/17	0.96	0.23	28,29,36,50	0
1	TRQ	D	697	16/17	0.97	0.19	28,29,44,46	0
1	TRQ	B	697	16/17	0.98	0.18	22,23,30,36	0
2	TRQ	C	697	16/17	0.98	0.21	23,24,29,35	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	902	5/5	0.78	0.38	98,104,109,120	0
5	PGE	B	907	10/10	0.80	0.27	44,93,111,121	0
3	SO4	B	905	5/5	0.85	0.24	84,96,110,113	0
3	SO4	C	903	5/5	0.86	0.33	88,97,116,126	0
3	SO4	B	903	5/5	0.91	0.21	89,92,104,105	0
3	SO4	B	904	5/5	0.91	0.22	85,89,100,112	0
3	SO4	A	902	5/5	0.92	0.36	111,115,117,121	0
6	GLY	D	905	5/5	0.92	0.22	48,79,111,111	0
3	SO4	A	901	5/5	0.93	0.21	66,91,106,112	0
6	GLY	A	905	5/5	0.93	0.20	46,84,123,123	0
4	MG	A	903	1/1	0.93	0.15	48,48,48,48	0
3	SO4	B	901	5/5	0.94	0.22	101,107,113,116	0
3	SO4	D	901	5/5	0.94	0.21	86,100,112,116	0
4	MG	C	904	1/1	0.95	0.18	34,34,34,34	0
3	SO4	C	901	5/5	0.95	0.17	82,82,96,110	0
6	GLY	A	904	5/5	0.96	0.18	33,45,49,63	0
3	SO4	B	902	5/5	0.96	0.17	76,78,90,109	0
6	GLY	D	904	5/5	0.96	0.20	41,53,71,71	0
3	SO4	C	902	5/5	0.96	0.18	70,76,94,100	0
4	MG	B	906	1/1	0.97	0.19	32,32,32,32	0
4	MG	D	903	1/1	0.97	0.20	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.